Residence Time Effects on Soot Growth Processes

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Soot growth processes affect both the radiative heat transfer distribution in a fire as well as the smoke properties. While it is difficult to achieve long residence time effects in laboratory scale flames at normal gravity, it is relatively easier to produce these conditions in microgravity flames. Within a novel microgravity burner configuration used by Atreya and coworkers[1] 2 and 3 seconds of residence time are achieved in a relatively small microgravity flame (cf. figure 1). We have performed computational and theoretical investigations of the soot growth processes within this geometry as well as investigations of the convective and radiative coupling on the total radiative transfer and burner characteristics [2,3].

By coupling the soot and gas phase chemistry with radiative heat transfer processes, detailed effects of radiation from both the soot and gas phase species on the kinetics can be examined in a quasi-steady state microgravity spherical acetylene-air diffusion flame. The gas phase reaction is modeled by either single step or two step chemical kinetics. The soot reaction mechanism includes nucleation, surface growth, oxidation and coagulation steps. The radiation from both soot and the gas phase are calculated by employing a spherical harmonics (P-1 approximation) model. The local Planck mean absorption coefficients of the computed species are specified in the computations.

As a benchmark for these calculations, figure 2 shows the computational soot mass as a function of time as compared with experimental data. Basic soot agglomeration models assume that soot aggregates into volume effective spheres which was shown in Ezekoye and Zhang [2] to predict a low soot specific surface area prediction. In figure 2 we contrast the predicted soot mass time history by assuming volume effective agglomeration and then by assuming no agglomeration at all. It is not surprising that the prediction based on the non-agglomerating assumption over-predicts the soot net growth rate. The finite connection area between soot primary particles ensures that the actual soot surface area is between these two limiting assumptions.

Figure 3 shows the calculated flame radius (defined by the maximum reaction rate) compared with experimental measurements by Atreya et al. There is relatively good agreement between the predicted flame radius and the experimentally measured radius. Two experimentally measured temperatures are compared with the calculated temperatures and are presented in figure 4. The surface area per unit volume in the absence of agglomeration achieves maximum values of approximately 50 cm^{-1} which compare favorably with the measurements of Dobbins et al.[4] where surface area per unit volume estimates are approximately 20 cm^{-1} . By not allowing the particles to agglomerate as spherical objects, the total number of primary particles within the system increases with time. Figure 5 presents the soot number density in mixture fraction space at various times and shows that in the flame region the number densities are significantly larger for the non-agglomerating mechanism, and that on the air side of the flame that the number densities are independent of the agglomeration model. Examination of figure 5 shows that the number of primary particles per aggregate increases from order 10 near the flame sheet to a maximum value of order 10,000 and then decreases to order 1 in the fuel rich region of the flame. These extremely large primary particle numbers (i.e., order 10,000) are consistent with recent soot morphology measurements by Ito et al. [5] in a micro-gravity diffusion flame suggesting that in the absence of strong convection (i.e., cases where the soot has long residence times) the number of soot primary particles per aggregate is significantly larger than in a normal gravity flame. Finally figure 6 presents the growth budget for this flame and shows the volume averaged contributors to the soot growth process as a function of time. For this particular flame, it is evident that only at very short times ($t < 0.1$ ms) does soot nucleation add mass to the soot mass at a larger rate than soot surface growth. For constant absorption coefficient conditions, soot oxidation by OH is always larger than soot oxidation by O_2, and at approximately 10 ms, soot oxidation begins to consume more mass than nucleation adds to the system. Finally, it is shown that only at very long times (approximately 1 second) is there a net decrease in soot mass associated with oxidation processes.

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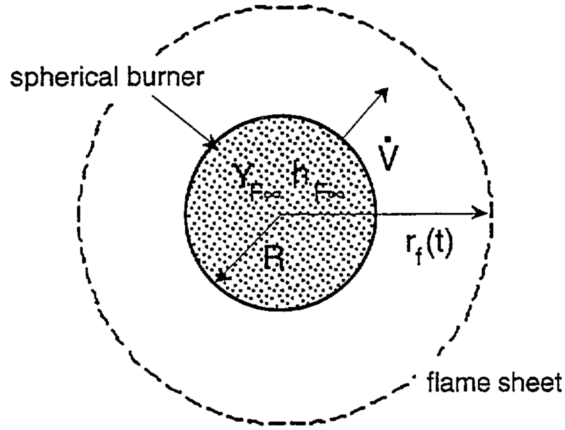

Fig.1 Schematic of computational domain

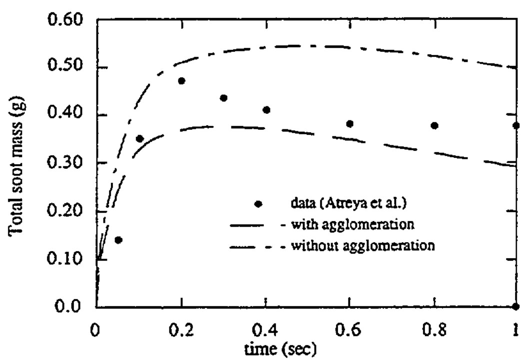

Fig.2 Soot mass predictions compared to expts.

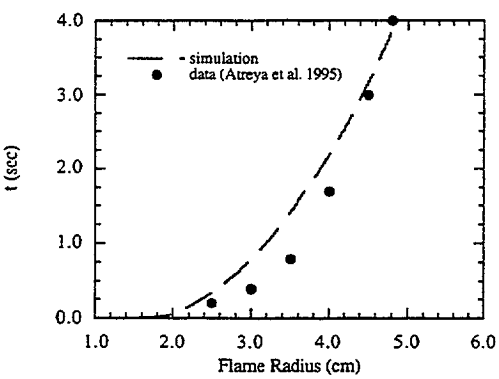

Fig. 3 Flame radius compared to expts.

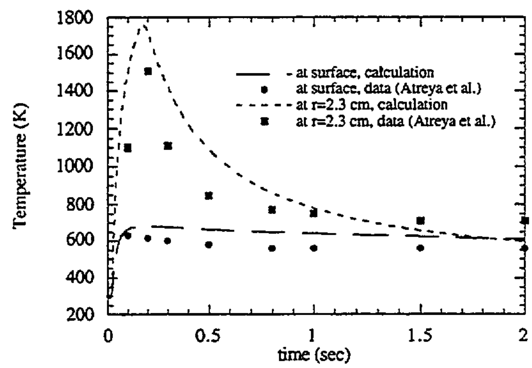

Fig. 4 Flame temperature predictions and expts.

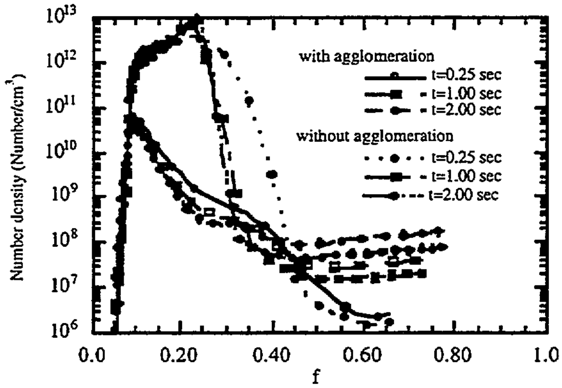

Fig. 5 Soot number concentration predictions

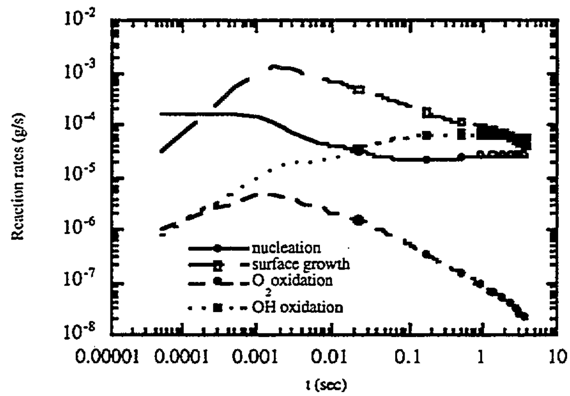

Fig. 6 Growth budget for soot species